

Green function theory of orbital magnetic moment of interacting electrons in solids

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(Dated: December 22, 2015)

A general formula for the orbital magnetic moment of interacting electrons in solids is derived using the many-electron Green function method. The formula factorizes into two parts, a part that contains the information about the one-particle band structure of the system and a part that contains the effects of exchange and correlations carried by the Green function. The derived formula provides a convenient means of including the effects of exchange and correlations beyond the commonly used local density approximation of density functional theory.

PACS numbers: 71.20.-b, 71.27.+a

The magnetic moment of an atom is composed of two components: one arises from the spins of the electrons and another from the orbital motion of the electrons around the nucleus. When atoms are assembled together to form a crystal, these magnetic moments originating from the individual atoms survive. Until recently, it was thought that calculating the magnetic moment of a crystal amounts to calculating the local magnetic moments of the constituent atoms. Some years ago, however, it was discovered that in addition to the contribution from the local atomic orbital moments there is a contribution emerging from the itinerant motion of the electrons on the surface of the crystal^{1,2}. In the thermodynamic limit when the system size becomes very large, this contribution does not depend on the geometry of the surface and can be expressed in terms of bulk quantities.

Although in many cases, the magnetic moment is dominated by the contribution from the electron spins, in some cases the contribution from the orbital moment can be significant. It is therefore important to have a rigorous formulation for calculating the orbital moment contribution to the total magnetic moment. It has been recognized for a long time that calculating the orbital magnetic moment of a crystal is a nontrivial task due to the infinite nature of a crystal that renders the position operator entering the expression for the orbital moment ill-defined^{3,4}. In this respect, the problem is akin to the calculation of the polarization of a crystal which was solved by King-Smith and Vanderbilt^{5,6} in the early nineties by utilizing Wannier orbitals and the Berry-phase approach⁷. A similar approach was proposed by Resta *et al*^{3,4} for calculating the orbital magnetic moment in crystals and led to the finding of the possible presence of an additional itinerant contribution which was put on a firm theoretical basis in a later work¹. Independently and parallel to the Wannier-orbital approach, a semiclassical method was proposed by Xiao *et al*² and later a linear-response technique by Shi *et al*⁹ to derive a general expression for the orbital magnetic moment of a crystal. A mathematically elegant derivation was also

presented very recently by Bianco and Resta¹⁰.

These pioneering works have opened up a way for computing the orbital magnetic moment of a crystal from realistic band structure calculations^{11,12}. The focus, however, has been on non-interacting systems represented by one-particle Bloch states and the corresponding eigenvalues usually obtained from the Kohn-Sham theory of density functional theory. For interacting systems, the subject is still new and unexplored. An extension to interacting systems was proposed within the framework of the current and spin density functional theory which provides an appealing analogue to the non-interacting formulation. While current and spin density functional theory is formally exact it is common practice to use the local density approximation for the exchange-correlation potential. However, it is hard to improve upon the local density approximation (LDA) in a systematic fashion.

In this letter, we present a general alternative method for calculating the orbital magnetic moment of interacting many-electron systems in a periodic lattice based on the many-body Green function technique. Green function method is rather well established and allows for a more systematic improvement compared with the density-functional based approaches. Indeed, in the last couple of decades there has been a number of important breakthroughs in applying it to calculate the electronic structure and spectroscopic properties of realistic materials. The *GW* approximation^{13–16} and the dynamical mean-field theory (DMFT)¹⁷ in combination with the LDA (LDA+DMFT) are prime examples of Green-function based theories successfully applied to real materials. These two methods provide effective tools for describing the electronic structure of materials from weakly to strongly correlated.

The orbital moment of a many-electron system is given by

$$\mathbf{M}_{\text{orb}} = \langle \Psi | \hat{\mathbf{L}} | \Psi \rangle \quad (1)$$

where Ψ is the many-electron ground state and the an-

gular momentum operator is given by

$$\hat{\mathbf{L}} = \int dr \hat{\psi}^\dagger(r) \mathbf{L}(r) \hat{\psi}(r), \quad \mathbf{L} = \mathbf{r} \times \mathbf{v}. \quad (2)$$

We use the notation $r = (\mathbf{r}, \sigma)$ and work in atomic unit ($\hbar = m = e = 1$) throughout the derivation. The magnetic moment is obtained by multiplying the orbital moment by a factor $-e/2c$ (Gaussian units). The velocity operator may be expressed as a commutator

$$\mathbf{v} = i[H, \mathbf{r}]. \quad (3)$$

H is a one-particle Hamiltonian whose eigenfunctions given by

$$H\psi_{\mathbf{k}n} = E_{\mathbf{k}n}\psi_{\mathbf{k}n} \quad (4)$$

may be chosen to define the field operator $\hat{\psi}$ in Eq. (2). For example, H is chosen in practice to be the Kohn-Sham Hamiltonian. We can express M_{orb} in terms of many-electron Green function as follows:

$$\mathbf{M}_{\text{orb}} = -i \lim_{r' \rightarrow r} \int dr \mathbf{L}(r') G^+(r', r), \quad (5)$$

$$G^+(r', r) = i \left\langle \Psi | \hat{\psi}^\dagger(r't) \hat{\psi}(r't) | \Psi \right\rangle. \quad (6)$$

We may expand the Green function in maximally localized Wannier orbitals^{18,19} $\{\varphi_{\mathbf{R}n}\}$ and to simplify writing we use a notation in which repeated indices are summed:

$$G^+(r', r) = \varphi_{\mathbf{R}'n'}(r') G_{\mathbf{R}'n', \mathbf{R}n}^+ \varphi_{\mathbf{R}n}^*(r) \quad (7)$$

where

$$\varphi_{\mathbf{R}n}(r) = \frac{1}{N} e^{-i\mathbf{k} \cdot \mathbf{R}} \tilde{\psi}_{\mathbf{k}n}(r), \quad \tilde{\psi}_{\mathbf{k}n}(r) = e^{i\mathbf{k} \cdot \mathbf{R}} \varphi_{\mathbf{R}n}(r), \quad (8)$$

$$\tilde{\psi}_{\mathbf{k}n}(r) = \psi_{\mathbf{k}m} S_{mn}(\mathbf{k}). \quad (9)$$

With the above definitions, $\varphi_{\mathbf{R}n}$ is normalized over the entire space whereas $\tilde{\psi}_{\mathbf{k}n}$ is normalized over the unit cell. The transformation matrix S_{mn} ensures that a given band labelled by n is smooth in the Wannier basis^{18,19}. The Wannier orbitals are used as a tool but the final formula for the orbital magnetic moments is expressed entirely in terms of Bloch states. In this work, we restrict ourselves to systems with zero Chern number since the above construction of Wannier orbitals may not be valid for systems with nonzero Chern number.

Using the Wannier expansion, the total orbital moment can be split into a local and an itinerant term:

$$\mathbf{M}^L = -i G_{\mathbf{R}'n', \mathbf{R}n}^+ \int dr \varphi_{\mathbf{R}n}^*(r) [(\mathbf{r} - \mathbf{R}) \times \mathbf{v}] \varphi_{\mathbf{R}'n'}(r), \quad (10)$$

$$\mathbf{M}^I = -i G_{\mathbf{R}'n', \mathbf{R}n}^+ \int dr \varphi_{\mathbf{R}n}^*(r) (\mathbf{R} \times \mathbf{v}) \varphi_{\mathbf{R}'n'}(r). \quad (11)$$

In the thermodynamic limit, when the system is made increasingly large, each atom labelled by \mathbf{R} contributes equally to \mathbf{M}^L and we may set $\mathbf{R} = \mathbf{0}$ and multiply by the number of atoms. We are assuming for simplicity that there is one atom per unit cell but extension to many atoms per unit cell is quite straightforward and the final formula is not affected by this assumption. The local orbital moment per unit volume is then

$$\mathbf{m}^L = -\frac{i}{\Omega} G_{\mathbf{R}'n', \mathbf{0}n}^+ \int dr \varphi_{\mathbf{0}n}^*(r) (\mathbf{r} \times \mathbf{v}) \varphi_{\mathbf{R}'n'}(r). \quad (12)$$

Eq. (12) has a clear physical interpretation: For $\mathbf{R}' = \mathbf{0}$ it corresponds to the rotation of the Wannier orbital around the origin. For $\mathbf{R}' \neq \mathbf{0}$ the Green function $G_{\mathbf{R}'n', \mathbf{0}n}^+$ is the probability amplitude for an electron at a Wannier orbital n located at the origin to hop to a Wannier orbital n' located at \mathbf{R}' . Multiplying it with the matrix element $\langle \varphi_{\mathbf{0}n} | \mathbf{r} \times \mathbf{v} | \varphi_{\mathbf{R}'n'} \rangle$ gives the contribution to the orbital moment from that electron that hops to $\varphi_{\mathbf{R}'n'}$. For a non-interacting system, the $\mathbf{R} = \mathbf{0}$ term in (12) corresponds to Eq. (16) of Thonhauser²⁰ and for an occupied band, it can be shown, assuming $S = 1$ and using

$$G_{n'n}^+(\mathbf{q}) = G_{\mathbf{R}'n', \mathbf{0}n}^+ e^{-i\mathbf{q} \cdot \mathbf{R}'} = i n_F(E_{\mathbf{q}n}) \delta_{n'n} \quad (13)$$

where n_F is the Fermi function, that the $\mathbf{R} \neq \mathbf{0}$ terms in Eq. (12) vanish but they may be finite for metallic systems.

The itinerant contribution \mathbf{M}^I for $\mathbf{R} = \mathbf{R}'$ and $n = n'$ is interpreted as arising from the center-of-mass motion of the Wannier orbitals $\varphi_{\mathbf{R}n}$ on the surface. The $\mathbf{R} \neq \mathbf{R}'$ and $n \neq n'$ terms describe an additional itinerant contribution from the possibility of hopping from $\varphi_{\mathbf{R}n}$ to $\varphi_{\mathbf{R}'n'}$.

We now express \mathbf{m}^L in terms of Bloch states. Using the commutator in Eq. (3) and the Levi-Civita symbol ϵ_{ijk} we find

$$m_i^L = \frac{1}{\Omega} G_{\mathbf{R}'n', \mathbf{0}n}^+ \epsilon_{ijk} \int dr \varphi_{\mathbf{0}n}^*(r) r_j H r_k \varphi_{\mathbf{R}'n'}(r) \quad (14)$$

where the other term arising from the commutator is zero since $\sum_{jk} \epsilon_{ijk} r_j r_k = 0$. Using the identity

$$r_k \varphi_{\mathbf{R}'n'}(r) = i \frac{\Omega}{(2\pi)^3} \int d^3 q' e^{i\mathbf{q}' \cdot \mathbf{r}} \frac{\partial}{\partial q'_k} [e^{-i\mathbf{q}' \cdot \mathbf{R}'} \tilde{u}_{\mathbf{q}'n'}(r)] \quad (15)$$

where $\tilde{u}_{\mathbf{q}n} = \exp(-i\mathbf{q} \cdot \mathbf{r})\tilde{\psi}_{\mathbf{q}n}$ is the periodic part of the Bloch function and Ω is the unit cell volume, we obtain

$$m_i^L = \epsilon_{ijk} \int_{BZ} \frac{d^3q}{(2\pi)^3} \left\{ G_{n'n}^+(\mathbf{q}) \left\langle \frac{\partial \tilde{u}_{\mathbf{q}n}}{\partial q_j} \middle| H(\mathbf{q}) \middle| \frac{\partial \tilde{u}_{\mathbf{q}n'}}{\partial q_k} \right\rangle + \frac{\partial G_{n'n}^+(\mathbf{q})}{\partial q_k} \left\langle \frac{\partial \tilde{u}_{\mathbf{q}n}}{\partial q_j} \middle| u_{\mathbf{q}m'} \right\rangle E_{\mathbf{q}m'} S_{m'n'}(\mathbf{q}) \right\}. \quad (16)$$

where the integration over the crystal momentum space has been reduced to the Brillouin zone (BZ) and

$$H(\mathbf{q}) = e^{-i\mathbf{q} \cdot \mathbf{r}} H(r) e^{i\mathbf{q} \cdot \mathbf{r}}, \quad (17)$$

$$G_{n'n}^+(\mathbf{q}) \doteq \sum_{\mathbf{R}} G_{\mathbf{R}n',0n}^+ e^{-i\mathbf{q} \cdot \mathbf{R}}. \quad (18)$$

We now consider the itinerant term in (11). We need to evaluate $\langle \varphi_{\mathbf{R}n} | \mathbf{V} | \varphi_{\mathbf{R}'n'} \rangle$, which can be done by inserting a complete set of states in between H and \mathbf{r} :

$$\begin{aligned} & \langle \varphi_{\mathbf{R}n} | \mathbf{V} | \varphi_{\mathbf{R}'n'} \rangle \\ &= i [\langle \varphi_{\mathbf{R}n} | H | \varphi_{\mathbf{R}''m} \rangle \langle \varphi_{\mathbf{R}''m} | \mathbf{r} | \varphi_{\mathbf{R}'n'} \rangle \\ & - \langle \varphi_{\mathbf{R}n} | \mathbf{r} | \varphi_{\mathbf{R}''m} \rangle \langle \varphi_{\mathbf{R}''m} | H | \varphi_{\mathbf{R}'n'} \rangle]. \end{aligned} \quad (19)$$

We may choose \mathbf{R}'' as the origin of the coordinate and measure all vectors with respect to \mathbf{R}'' . Since the sums over \mathbf{R} and \mathbf{R}' run over all lattice points, we may relabel $\mathbf{R} - \mathbf{R}'' \rightarrow \mathbf{R}$ and $\mathbf{R}' - \mathbf{R}'' \rightarrow \mathbf{R}'$. Both H and G are not affected by the relabelling since they are periodic. We then find

$$\begin{aligned} \mathbf{M}^I &= -i G_{\mathbf{R}'n',\mathbf{R}n}^+(\mathbf{R} + \mathbf{R}'') \times \\ & i [\langle \varphi_{\mathbf{R}n} | H | \varphi_{\mathbf{0}m} \rangle \langle \varphi_{\mathbf{0}m} | \mathbf{r} + \mathbf{R}'' | \varphi_{\mathbf{R}'n'} \rangle \\ & - \langle \varphi_{\mathbf{R}n} | \mathbf{r} + \mathbf{R}'' | \varphi_{\mathbf{0}m} \rangle \langle \varphi_{\mathbf{0}m} | H | \varphi_{\mathbf{R}'n'} \rangle]. \end{aligned} \quad (20)$$

The terms containing \mathbf{R}'' can be shown to vanish because $\mathbf{R}'' \times \mathbf{R}'' = 0$ and for every \mathbf{R}'' there is $-\mathbf{R}''$. We then obtain, writing explicitly the sum over \mathbf{R}'' ,

$$\begin{aligned} \mathbf{M}^I &= -i \sum_{\mathbf{R}''} G_{\mathbf{R}'n',\mathbf{R}n}^+ \mathbf{R} \times \\ & i [\langle \varphi_{\mathbf{R}n} | H | \varphi_{\mathbf{0}m} \rangle \langle \varphi_{\mathbf{0}m} | \mathbf{r} | \varphi_{\mathbf{R}'n'} \rangle \\ & - \langle \varphi_{\mathbf{R}n} | \mathbf{r} | \varphi_{\mathbf{0}m} \rangle \langle \varphi_{\mathbf{0}m} | H | \varphi_{\mathbf{R}'n'} \rangle]. \end{aligned} \quad (21)$$

As can be seen, the expression under the summation over \mathbf{R}'' does not depend on \mathbf{R}'' so that the sum may be replaced by the number of sites N . The itinerant part of the orbital moment per unit volume is then

$$\begin{aligned} \mathbf{m}^I &= \frac{1}{\Omega} G_{\mathbf{R}'n',\mathbf{R}n}^+ \mathbf{R} \\ & \times [\langle \varphi_{\mathbf{R}n} | H | \varphi_{\mathbf{0}m} \rangle \langle \varphi_{\mathbf{0}m} | \mathbf{r} | \varphi_{\mathbf{R}'n'} \rangle \\ & - \langle \varphi_{\mathbf{R}n} | \mathbf{r} | \varphi_{\mathbf{0}m} \rangle \langle \varphi_{\mathbf{0}m} | H | \varphi_{\mathbf{R}'n'} \rangle], \end{aligned} \quad (22)$$

Using Eq. (15) we find

$$\langle \varphi_{\mathbf{0}m} | r_k | \varphi_{\mathbf{R}'n'} \rangle = -i \frac{\Omega}{(2\pi)^3} \int d^3q e^{-i\mathbf{q} \cdot \mathbf{R}} \left\langle \frac{\partial \tilde{u}_{\mathbf{q}m}}{\partial q_k} \middle| \tilde{u}_{\mathbf{q}n'} \right\rangle, \quad (23)$$

where we have used the fact that $\tilde{u}_{\mathbf{q}n}$ is periodic. The matrix element of the Hamiltonian can be written as

$$\langle \varphi_{\mathbf{R}n} | H | \varphi_{\mathbf{0}m} \rangle = \frac{\Omega}{(2\pi)^3} \int_{BZ} d^3q e^{i\mathbf{q} \cdot \mathbf{R}} \tilde{E}_{nm}(\mathbf{q}), \quad (24)$$

$$\tilde{E}_{nm}(\mathbf{q}) = \sum_{m'} S_{nm'}^\dagger(\mathbf{q}) E_{\mathbf{q}m'} S_{m'm}(\mathbf{q}). \quad (25)$$

Using the above two results and using the formula $\sum_{\mathbf{R}} \exp(i\mathbf{q} \cdot \mathbf{R}) = \delta(\mathbf{q})(2\pi)^3/\Omega$, as well as recognizing the fact that for a periodic system $G_{\mathbf{R}'n',\mathbf{R}n}^+$ depends on $\mathbf{R}' - \mathbf{R}$, the final result for the itinerant contribution is

$$\begin{aligned} m_i^I &= \epsilon_{ijk} \int_{BZ} \frac{d^3q}{(2\pi)^3} G_{n'n}^+(\mathbf{q}) \\ & \left[\left\langle \frac{\partial \tilde{u}_{\mathbf{q}n}}{\partial q_j} \middle| \frac{\partial \tilde{u}_{\mathbf{q}m}}{\partial q_k} \right\rangle \tilde{E}_{mn'}(\mathbf{q}) + \frac{\partial \tilde{E}_{nm}(\mathbf{q})}{\partial q_j} \left\langle \frac{\partial \tilde{u}_{\mathbf{q}m}}{\partial q_k} \middle| \tilde{u}_{\mathbf{q}n'} \right\rangle \right] \end{aligned} \quad (26)$$

This together with Eq. (16) constitute our main results. Unlike the non-interacting case with no band crossings for which G is diagonal in the band index, the summation over the band indices involves both intra- and inter-band matrix elements, reflecting the possibility of mixing between different bands when the interaction among the electrons is switched on or when there are band crossings. It is noteworthy that from perturbation theory we have⁸

$$\left| \frac{\partial u_{\mathbf{q}n}}{\partial q_i} \right\rangle = \sum_{m \neq n} \frac{|u_{\mathbf{q}m}\rangle \langle u_{\mathbf{q}m} | v_i | u_{\mathbf{q}n}\rangle}{E_{\mathbf{q}m} - E_{\mathbf{q}n}} \quad (27)$$

so that $\left\langle \frac{\partial u_{\mathbf{q}n}}{\partial q_i} \middle| u_{\mathbf{q}n'} \right\rangle = 0$ if $n' = n$.

Our formula for the orbital moment factorizes into two parts: the one-particle part, expressed by $u_{\mathbf{q}n}$ and $E_{\mathbf{q}n}$, contains information about the underlying band structure of the system whereas the interacting part, carried by the Green function, contains information about exchange and correlations of the interacting electrons.:

$$G^{-1} = G_0^{-1} - \Sigma \quad (28)$$

where Σ is the self-energy and G_0 is a non-interacting Green function expressed in terms of $u_{\mathbf{q}n}$ and $E_{\mathbf{q}n}$. The formula is quite general and provides a convenient means of including the effects of exchange and correlations through the many-electron Green function. It goes

over into the non-interacting formula as the self-energy is switched off. As pointed out earlier, our derived formula for the orbital magnetic moment is only valid for systems with zero Chern number, where the Bloch orbitals always can be chosen to be smooth and obey the periodic gauge $\psi_{\mathbf{k}n} = \psi_{\mathbf{k}+\mathbf{G},n}$. However, when the Chern number becomes nonzero, the periodic gauge is no longer valid. As a consequence integrals around the perimeter of the Brillouin zone will not vanish; there will be contributions due to singularities located in the interior of the Brillouin zone²¹.

Let us now apply our formula to a non-interacting insulating system without band crossing in which case the transformation matrix $S = 1$. In this case G is diagonal in the band index and $\left\langle \frac{\partial u_{\mathbf{q}n}}{\partial q_i} | u_{\mathbf{q}n'} \right\rangle = 0$ if $n' \neq n$ and we obtain

$$m_i = -\epsilon_{ijk} \int \frac{d^3q}{(2\pi)^3} n_F(E_{\mathbf{q}n}) \times \text{Im} \left\langle \frac{\partial u_{\mathbf{q}n}}{\partial q_j} \left| H(\mathbf{q}) + E_{\mathbf{q}n} \right| \frac{\partial u_{\mathbf{q}n}}{\partial q_k} \right\rangle, \quad (29)$$

multiplying by $-e/2c$ (Gaussian units) to obtain the magnetic moment. This result is in agreement with that in Refs.^{1,2,8}. We have also applied this formula to the Haldane model²² and found good numerical agreement with previous calculations^{1,2,8}. When there are band crossings, S may not be a unit matrix anymore and consequently the formulas in Eqs. (16) and (26) may yield

additional contribution not included in the previous results.

In summary, we have derived a general formula for the orbital magnetic moment of interacting electrons in solids in which the effects of exchange and correlations are embodied in the many-electron Green function. The derivation does not rely on the presence of surface but simply makes use of the translational property of the lattice. By expanding the Green function in Wannier orbitals constructed from the underlying one-particle Bloch states of the system a seamless connection with the non-interacting formula is achieved. The Wannier orbitals are used only as a tool and the final formula is expressed entirely in terms of the Bloch states and the many-electron Green function written in the Bloch basis. The use of the Green function allows for a transparent physical interpretation of the formula. The formula provides a convenient access to inclusion of exchange and correlations beyond the commonly used local density approximation. For example, the self-energy needed in Eq. (28) can be calculated using the standard GW approximation for weakly to moderately correlated materials and the LDA+DMFT or the recently developed GW +DMFT²³, in the case of systems with strong onsite correlations.

Acknowledgments

We would like to thank K. Terakura for valuable comments and discussions during the course of this work. This work was partly supported by the Swedish Research Council.

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